NATIONAL ENERGY TECHNOLOGY LABORATORY

Carbon Dioxide Capture Research

NETL Office of Research and Development

Status and Directions

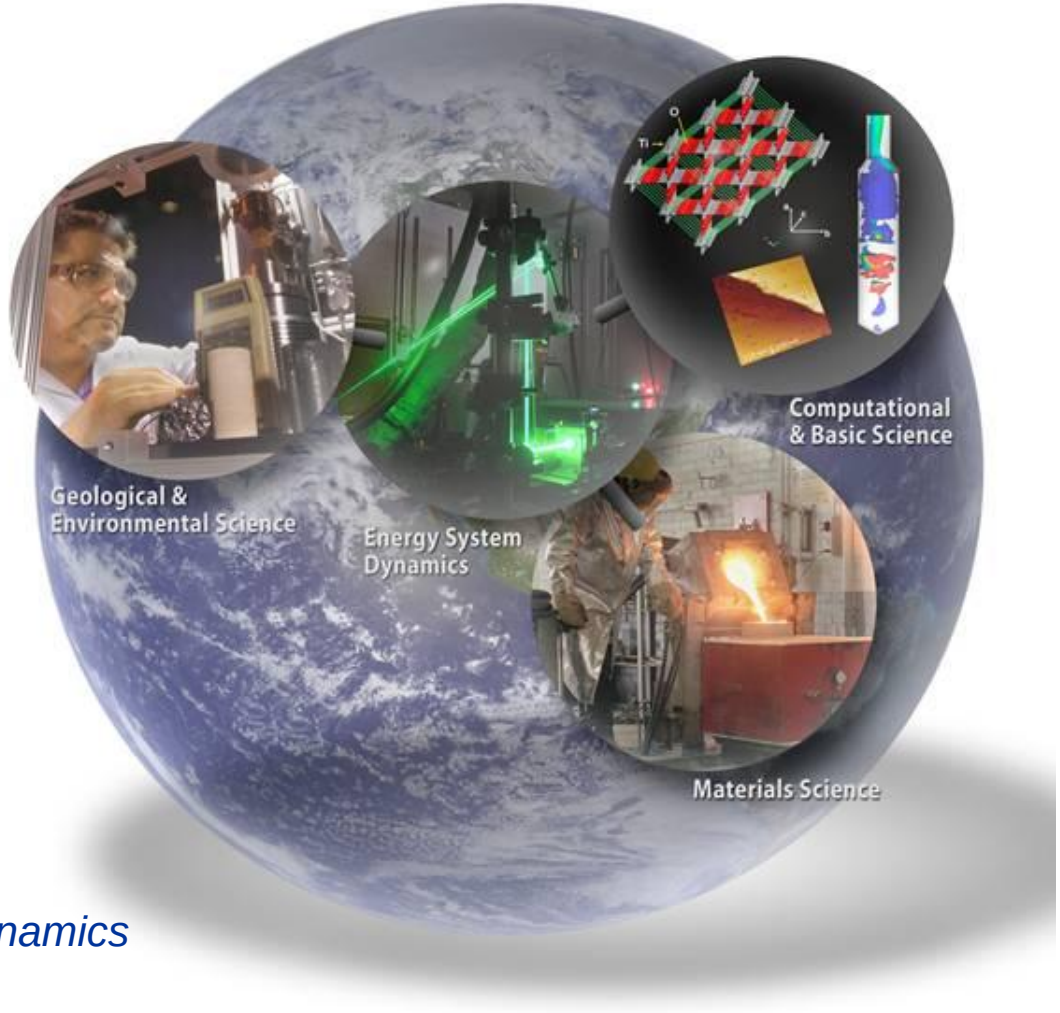
The contributions of numerous NETL staff are gratefully recognized.

Research and Development Focus Areas

Projects are Organized Across Area Expertise

George Guthrie
Geological & Environmental Science

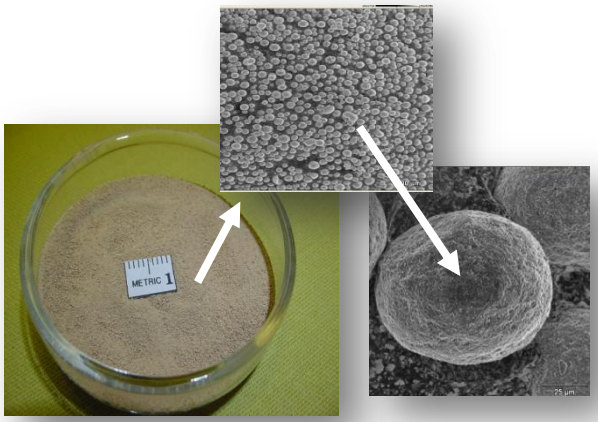
Madhava Syamlal
Compuational & Basic Science



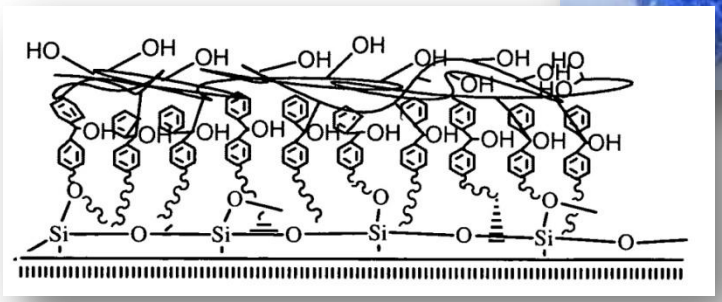
Geo Richards
Energy System Dynamics

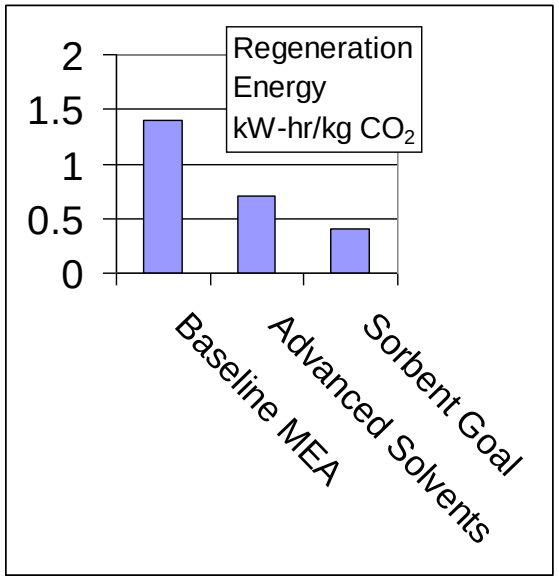
Cindy Powell
Materials Science

Dry CO_2 Sorbents



Numeric simulation of reactor concept for solid sorbents

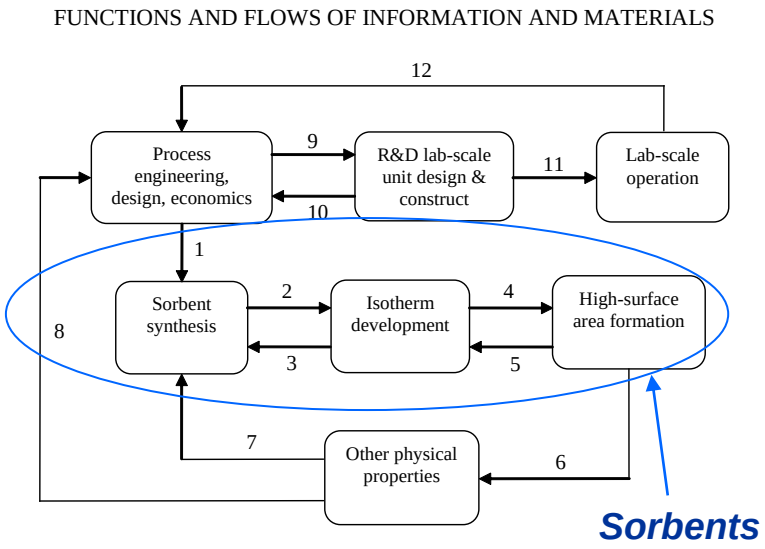


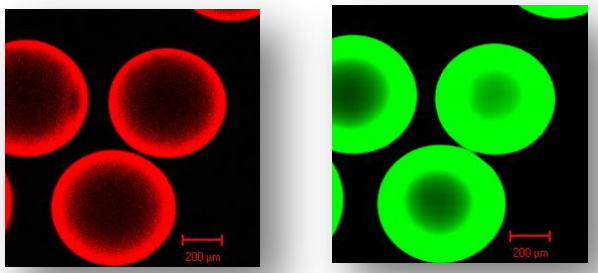


Progress on Solid Sorbents for CO_2

Development of three sorbent types, amine-based, plus new types

1. **Clay substrate (2009 R&D 100 Award)**
   - Expected low cost, easy to manufacture.
   - Ready for long-term tests and incorporation in detailed analysis.
2. **Polymer substrate**
   - Reasonable cost
   - Moisture effects are significant
   - Demonstrated nano-bio technique to create high-surface area film.
3. **Silica substrate**
   - Demonstrated good capacity, reduction in water effects, detailed quantification in progress.
   - Potential for higher temperature regeneration (120 °C) and with pure CO_2
4. **Revolutionary (ongoing and 2010 plan)**
   - Projects with EFRC being discussed
   - Supported Amino Acids
   - Computational screening



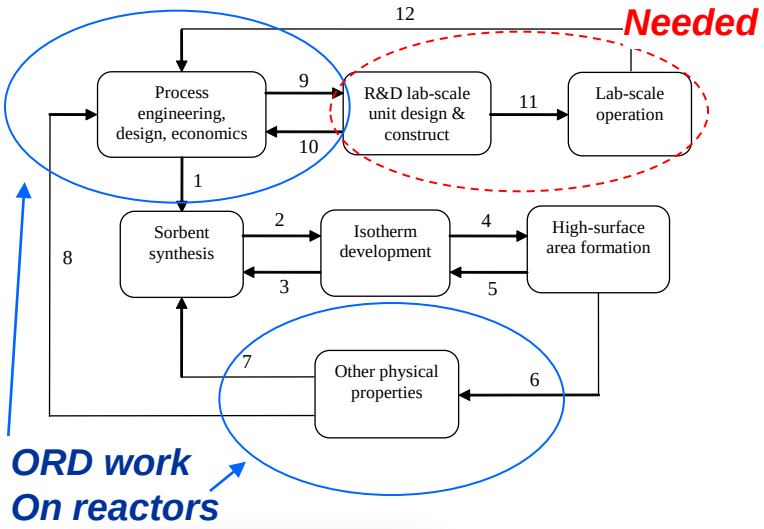


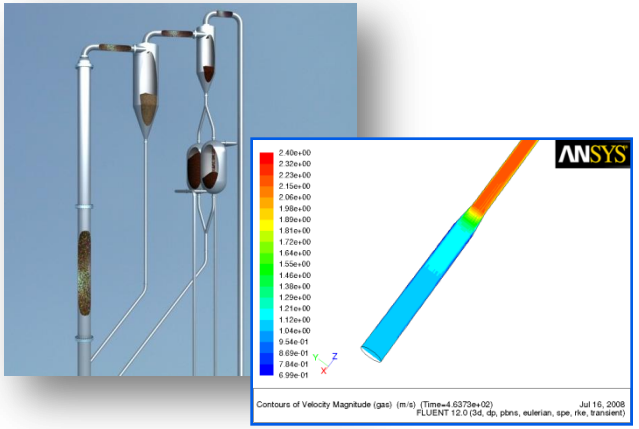
Schematic shows how layers (red/green & black) are deposited. Experimental deposition on 600 micron porous spheres showing "tagged" red/green adsorbent Deposition via confocal fluorescence microscopy.

Reactors for CO_2 Dry Sorbents

- **Initial/conceptual analysis of five reactor systems to use sorbents:**
  - Structured Bed Concept
    - Fixed bed sorber, with internal heat removal
    - Internal heating of same bed for regeneration
  - Moving Bed Concept
    - Moving bed sorber, with internal heat removal
    - Moving bed regenerator, with internal heating
  - Fluidized Bed Concept
    - Fluid bed sorber, with internal heat removal
    - Moving bed regenerator, with internal heating
  - Fixed Bed Adsorber Concept
    - Fixed bed sorber, adiabatic, multi-stage with interstage heat removal
    - Heating of same bed for regeneration with hot fluid stream
  - Transport Reactor
    - Circulating fluid bed sorber
    - Circulating fluid or moving bed regenerator

FUNCTIONS AND FLOWS OF INFORMATION AND MATERIALS

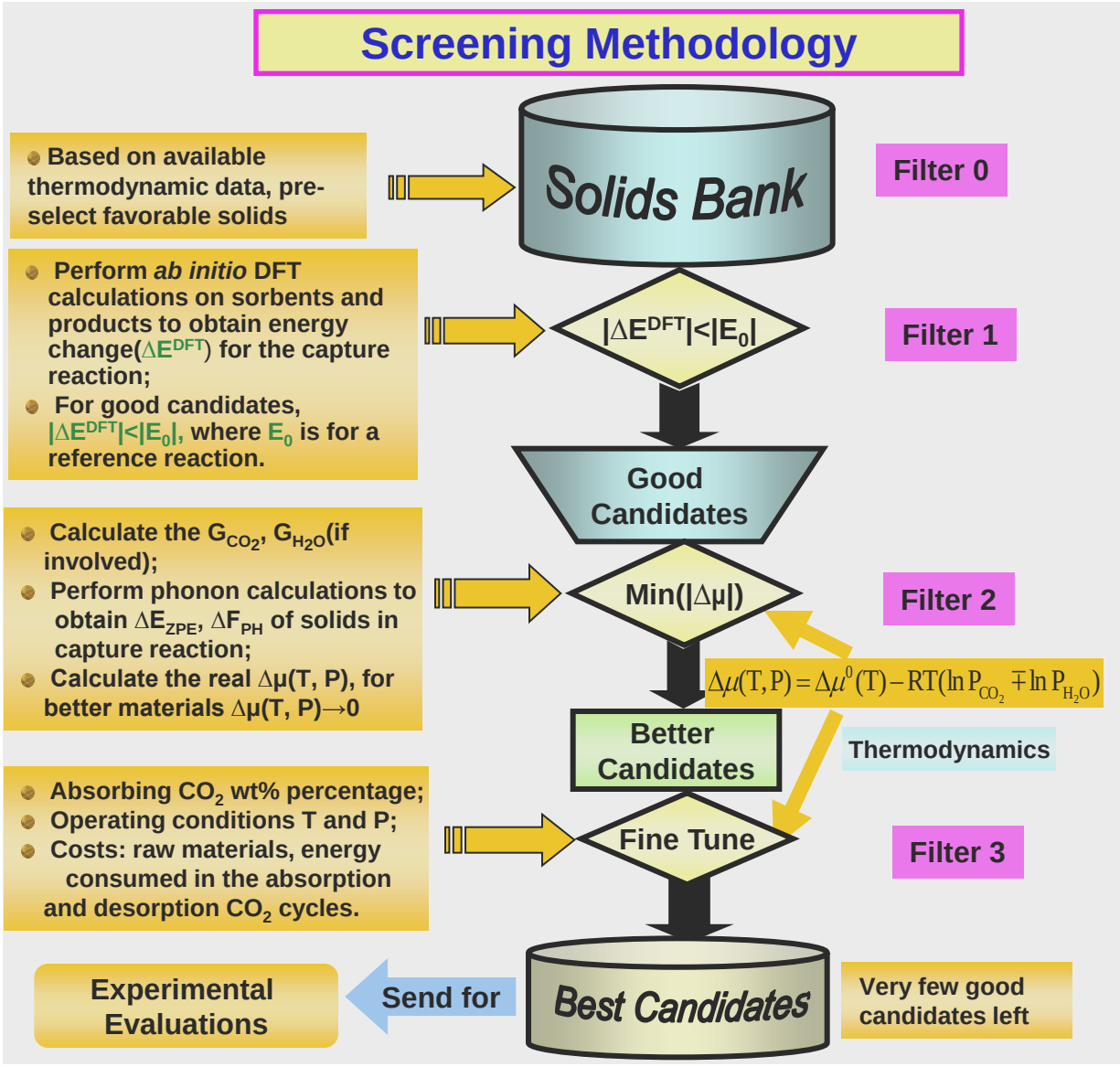




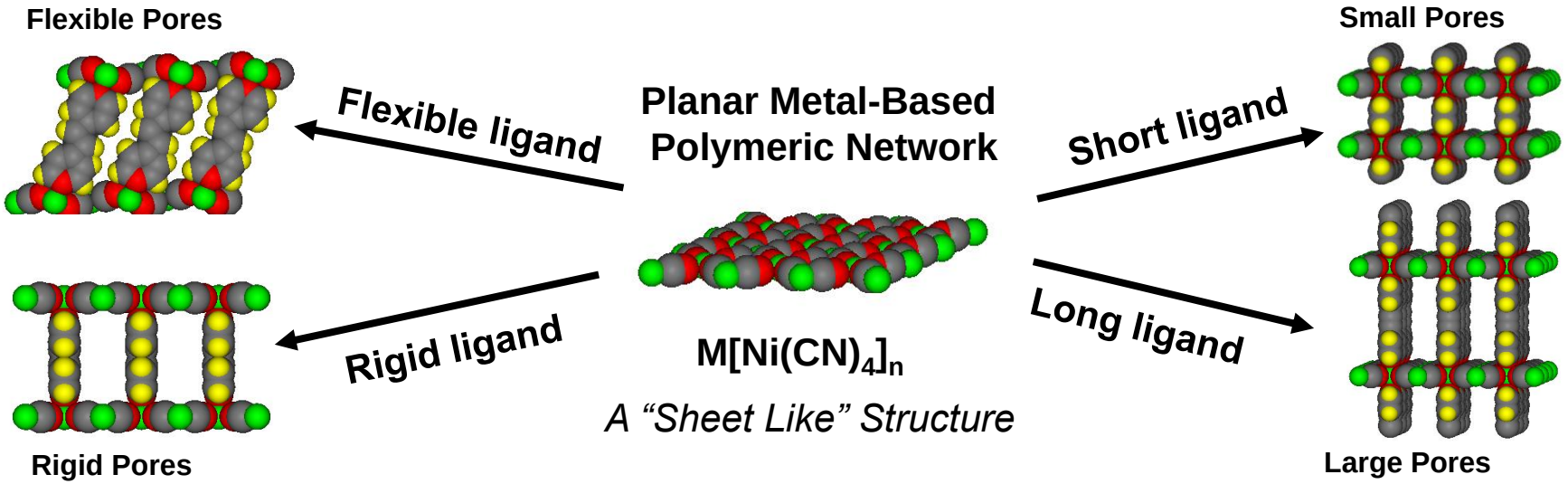
Computational Screening of CO_2 Solid Sorbents

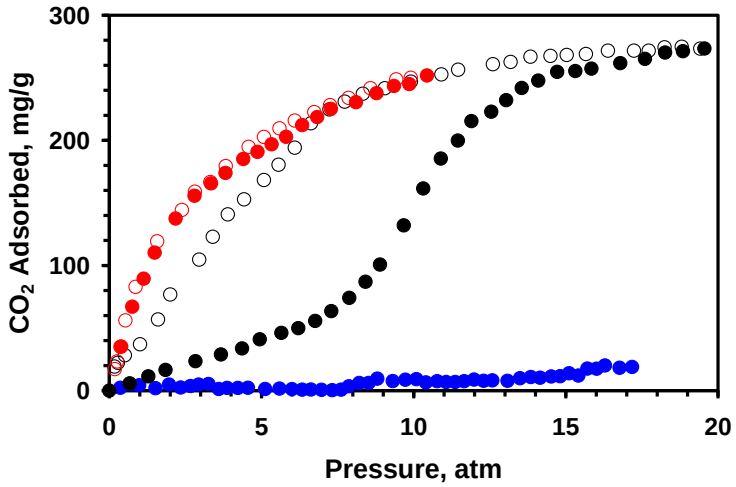
- Thermodynamic properties of CO_2 sorbents determined by combining density functional theory with lattice phonon calculations
- Candidate sorbents selected by applying several filters
- Validated the method by comparing predicted thermodynamic properties of many simple oxides, salts and hydroxides with experimental data
- More than 200 compounds have been investigated
- Several promising candidates were recommended for experimental investigation
- This methodology allows us to explore new sorbent materials, such as composites, mixtures, substituted and doped systems, for which thermodynamic properties are unknown.

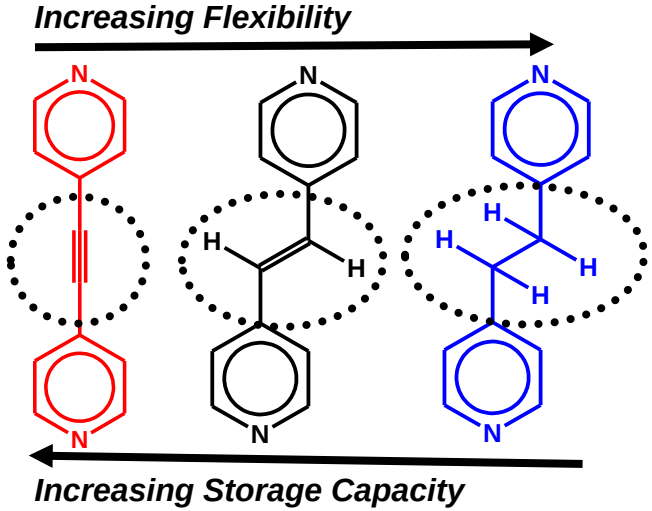
Y. Duan, *Proc. 7th and 8th Annual Conf. on Carbon Capture & Sequestration*, 2008, 2009



Porous Coordination Polymers





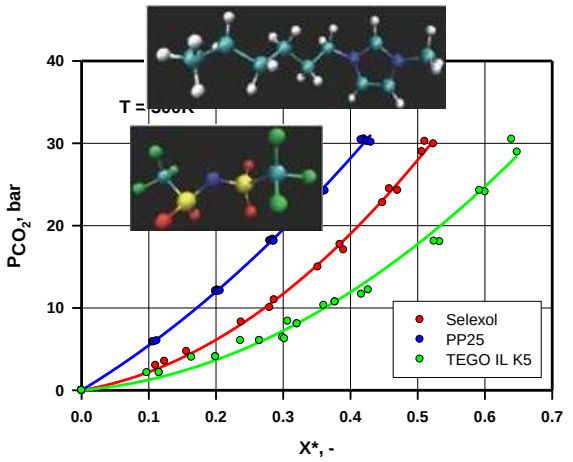


Applications

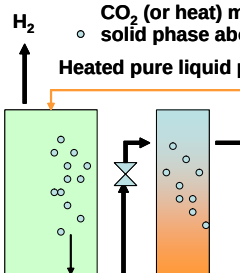
- CO_2 Capture
- H_2 Storage
- Gas Separations
- Validation of Computational Models

Pre-combustion Carbon Capture

- **Ionic Liquids – tailored CO_2 solvents**
  - Molecular Dynamics Simulation of Transport and Thermodynamic Properties
  - Computationally-guided Screening of CO_2 Sorption Capacity and Kinetic Parameters
  - Development of Membrane Fiber Support
- **Solids CO_2 sorbents for syngas**
  - With water-gas-shift for enhanced H_2 production
  - Reactor configuration/studies in progress
  - New phase-change polymers (solid → liquid)
- **Novel concepts**
  - CO_2 re-use opportunities–including photocatalytic reduction



Ionic liquid CO_2 capacity (green) versus other solvents (blue/red)



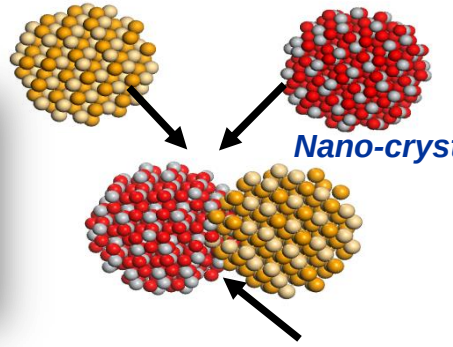
Concept for syngas CO_2 Capture w/phase change polymer

CO_2 membrane disk test and fiber bundle

Syngas CO_2 sorbent and test reactor

TiO_2 ***Photocatalyzes; won't absorb visible***

CdSe ***Absorbs visible light***



Nano-crystals

CO_2 photo-reduction occurs here. Demonstrated in NETL labs.

Oxy-Fuel Combustion

Enabling New or Retrofit Capture Power Plants

Background

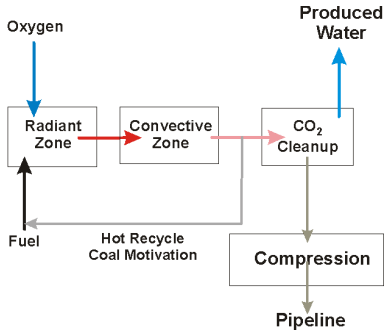
- Oxy-fuel simplifies CO_2 separation
- Replaces air (O_2 + N_2) with (O_2 + CO_2-recycled)
- New issues for combustion, heat transfer, CO_2 purification, materials

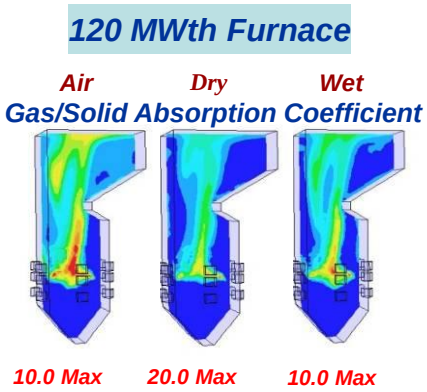
Research

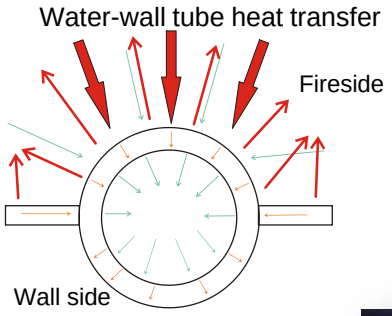
- Develop models for combustion, radiation, heat transfer
- Investigate methods to integrate CO_2 purification with thermal cycle
- Evaluate material performance in existing (600 °C)/advanced (760 °C) steam cycles

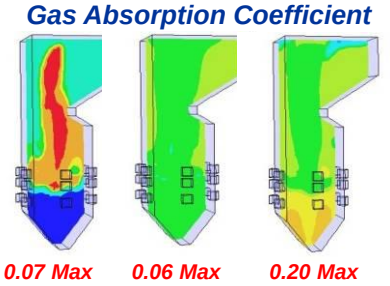
Status

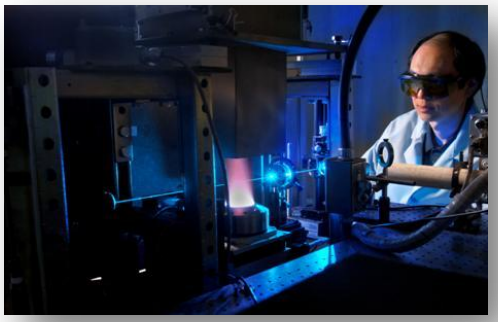
- Grey-gas radiation model and particle model under development
- Fireside corrosion test: exposure tests with ash and flue gas; oxide fluxing behavior in ash and flue gas
- Integrated Pollutant Removal (IPR) licensed
- Flame emissions and heat transfer measurements in boilers











Chemical Looping

Inherent CO_2 Capture for Power/Chemical Production

Background

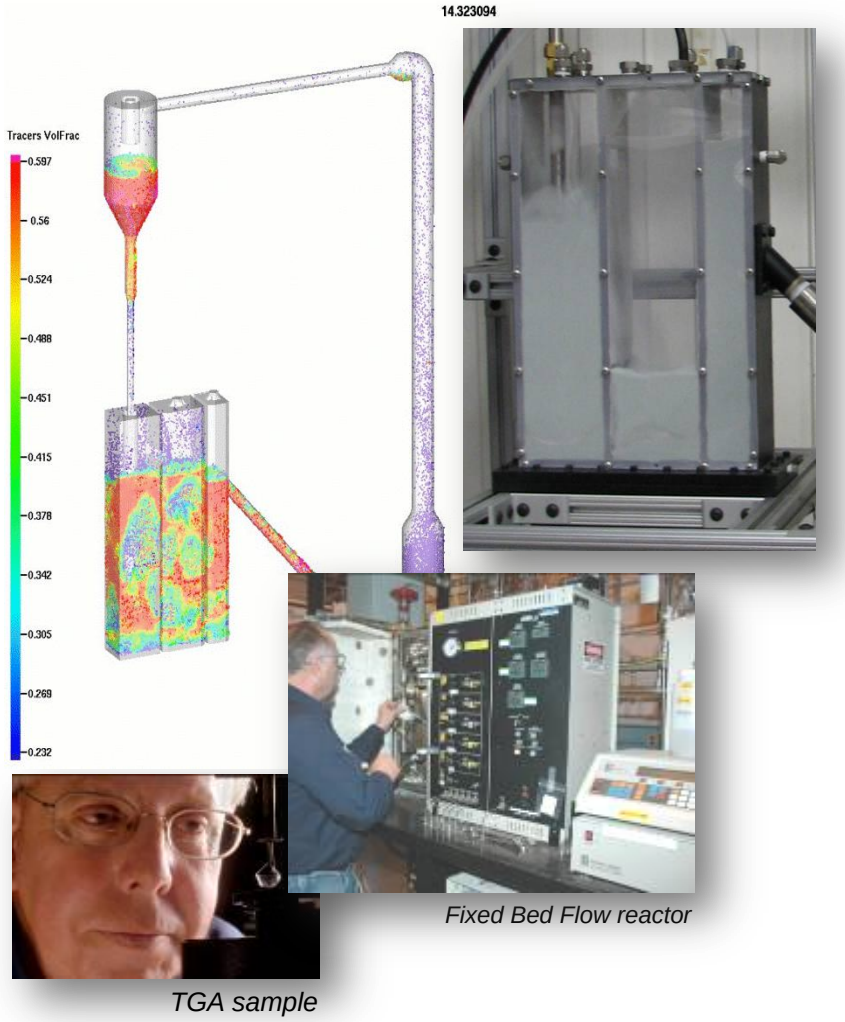
- Carbon + metal oxide = CO_2 + metal
- H_2O + metal = H_2 + metal oxide

Research

- Develop “oxygen carriers”
- Devise solids handling for ash separation
- Evaluate process concepts
- Dynamic models for control

Status

- Demonstrated oxygen carrier performance (size, composition, substrate)
- Simulation of reactor beds
- Tests of ash separation



Fixed Bed Flow reactor

TGA sample

Coal + MeO = CO_2 +water + heat ….w/o steam input

High-Fidelity Design of Advanced Energy Processes

Process/Equipment Co-Simulation and Optimization for Carbon Capture

Background

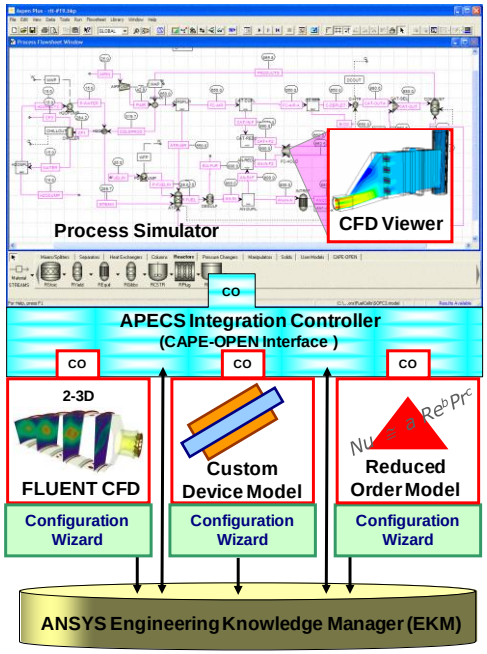
- Need tools for meeting aggressive design, environmental, and cost goals for advanced energy systems

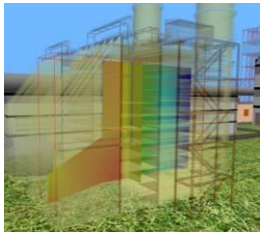
Research

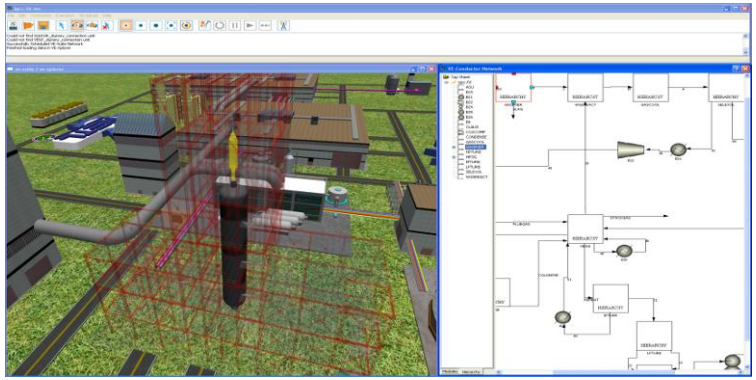
- Develop high-fidelity process and equipment co-simulation
- Provide seamless data/model management throughout the power plant lifecycle
- Develop virtual plant co-simulation capabilities

Status

- Advanced Process Engineering Co-simulator (APECS) - 2004 R&D100 Award
- APECS with ANSYS® EKM® - 2008 R&D100 Award
- APECS with VE-Suite (VE-PSI) - 2009 R&D100 Award







Summary

- **NETL-ORD is investigating multiple concepts for CO_2 capture**
  - Flue gas sorbents
  - Chemical looping
  - Oxy-fuel combustion
  - Pre-combustion membranes, sorbents
  - CO_2 re-use concepts are under investigation
- **A combination of applied science tools and engineering science are being used:**
  - Computational chemistry through system models.
  - Surface science through material science.
- **Significant opportunities exist to coordinate BES advances with Fossil applications.**